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A second-order, uniquely solvable, energy stable BDF numerical scheme for the phase field crystal model

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ABSTRACT

In this paper, we propose a second-order time accurate convex splitting scheme for the phase field crystal model. The temporal discretization is based on the second-order backward differentiation formula (BDF) and a convex splitting of the energy functional. The mass conservation, unconditionally unique solvability, unconditionally energy stability and convergence of the numerical scheme are proved rigorously. Mixed finite element method is employed to obtain the fully discrete scheme due to a sixth-order spatial derivative. Numerical experiments are presented to demonstrate the accuracy, mass conservation, energy stability and effectiveness of the proposed scheme.

1. Introduction

The phase field crystal (PFC) model was proposed by Elder et al. [7,8] as a powerful approach for modeling and predicting mesoscale morphological and microstructural evolution in materials by introducing a free energy functional of the local-time-averaged density field, where the crystal/liquid interface is considered as a transition layer over which a continuous, but steep changes of some physical quantities (such as concentration, density, magnetization, etc.) occur. The PFC model, which is a dynamic equation of the density field, can be derived by minimizing the free energy functional. And this model can account for elastic and plastic deformations [9,10], dislocations [3], grain boundaries [22], multiple crystal orientations, and many other observable phenomena, see, e.g., [20] for a review.

Consider a dimensionless spatial free energy functional of Swift–Hohenberg type [7,8,23]

$$E(\phi) = \int_{\Omega} \left(\frac{1}{4}\phi^4 + \frac{1-\epsilon}{2}\phi^2 - |\nabla\phi|^2 + \frac{1}{2}(\Delta\phi)^2 \right) d\mathbf{x}, \tag{1.1}$$

where $\phi : \Omega \subset \mathbb{R}^d (d = 2, 3) \to \mathbb{R}$ is the density field and $\epsilon < 1$ is a small positive bifurcation constant with physical significance. The dynamic equations, for example, Swift–Hohenberg (SH) equation, phase field crystal (PFC) equation and modified phase field crystal (MPFC) equation, derived as a gradient flow of the free energy, admit an energy dissipation law which justifies its thermodynamic consistency and leads to a mathematically well-posed model. Additionally, the presence of the energy law serves as a guideline for the design of energy stable numerical schemes. Therefore, it is especially desirable to design numerical schemes that preserve the energy dissipation law at the discrete level. On one hand, the preservation of

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the energy law has been a criterion to judge the success of the numerical schemes to capture the correct long time dynamics of the system. On the other hand, the unconditional stability of the energy-law preserving scheme provides flexibility for dealing with the stiffness issue in phase field models. In particular, the dynamics of the coarse-graining (macroscopic) process may undergo rapid changes near the interface, so the non-compliance of energy dissipation laws may lead to spurious numerical solutions if the grid and time step sizes are not carefully chosen.

Recently, there have been a lot of numerical analysis works on the development of energy stable schemes for solving the PFC model. In [16,26], the authors proposed first- and second-order convex splitting finite difference schemes for solving the PFC model. A detailed convergence analysis for the fully discrete scheme formulated in [16] was provided in a recent work [6]. Zhang et al. [30] developed unconditionally energy stable schemes coupled with an adaptive time stepping strategy for long time simulations of the PFC model. In [28], Yang and Han applied the "Invariant Energy Quadratization" approach (see [14,29,31]) to solve the PFC model, and a series of efficient linear schemes were developed based on the first-order Euler method, the second-order BDF and the second-order Crank–Nicolson method, respectively. Glasner et al. [11] proposed a linear, second-order time accurate and unconditionally gradient stable method based on linear convex splitting. Gomez et al. [12] proposed a nonlinear, second-order time accurate, and unconditionally gradient stable method with the modified Crank–Nicolson method, which is not based on the convex splitting. In [13], a local discontinuous Galerkin method and some high order unconditionally energy stable schemes were presented. Dehghan and Mohammadi [5] used a semi-implicit method for the PFC and MPFC equations, which split the linear terms into backward and forward pieces while treating the nonlinear term explicitly. Vignal et al. [24] proposed a second-order finite element scheme based on a new splitting of energy.

Generally, the ways to split the energy functional are not unique, for example

- convex splitting (CS-1)

$$E^c(\phi) = \int_\Omega \left(\frac{1}{4}\phi^4 + \frac{1-\epsilon}{2}\phi^2 + \frac{1}{2}(\Delta\phi)^2 \right) d\mathbf{x}, \quad E^e(\phi) = \int_\Omega |\nabla\phi|^2 d\mathbf{x}, \tag{1.2}$$

- convex splitting (CS-2)

$$E^c(\phi) = \int_\Omega \left(\frac{1}{4}\phi^4 + \frac{1}{2}\phi\,(1+\Delta)^2\,\phi \right) d\mathbf{x}, \quad E^e(\phi) = \int_\Omega \frac{\epsilon}{2}\phi^2 d\mathbf{x}, \tag{1.3}$$

where, $E^c(\phi)$ is contractive term and $E^e(\phi)$ is expansive term. Here $(1+\Delta)^2 = 1+2\Delta+\Delta^2$. Obviously, $E^c(\phi) - E^e(\phi) = E(\phi)$. In [1,2,16,25,26], first- and second-order energy stable methods for the PFC and MPFC equation were proposed based on the CS-1, and in which the second-order time discrete schemes were established based on Crank–Nicolson method. Based on the CS-2, Shin and Lee et al. [17,21] presented first- and second-order energy stable schemes for the PFC and MPFC equations, in which the second-order time discrete schemes were also constructed based on Crank–Nicolson method. And the authors numerically compared the two splitting methods mentioned above and observed that both methods CS-1 and CS-2 have the same order of convergence, but the methods CS-2 are more accurate than the methods CS-1, from the perspective of error constant and numerical dissipation.

In this paper, we propose and analyze an alternate second-order energy stable scheme for the PFC model (2.8), based on convex splitting CS-2 and the second-order BDF temporal approximation framework, instead of the Crank–Nicolson one. Following the idea presented in the recent work [27] for Cahn–Hilliard equation, a second-order BDF 3-point stencil is used for the approximation of temporal derivative, the contractive term is updated implicitly for its strong convexity, and a second-order accurate, explicit extrapolation formula is used for the approximation of the expansive term. Such a structure makes the numerical scheme uniquely solvable and mass conservative. In addition, to ensure the energy stability of the numerical scheme, we need to add a second-order Douglas–Dupont regularization, in the form of $-A\tau\Delta(u^{k+1}-u^k)$. We prove that, under a mild requirement $A \geq \frac{\epsilon^2}{16}$, the BDF scheme is unconditionally energy stable, namely, no scaling law is needed between the time step τ and the spatial grid size h to ensure its validity. Moreover, with the help of Sobolev embedding $H^1(\Omega) \hookrightarrow L^6(\Omega)$, we prove the convergence of the proposed time discrete scheme.

For the PFC model, being a nonlinear, sixth-order partial differential equation in space, mixed formulation can be employed to reduce the continuity requirements to standard C^0 spaces used in traditional finite element methods. This work makes use of a mixed finite element method for space approximation, where the system that is solved involves a coupled system of three second-order equations.

The paper is organized as follows. In the next section, the governing equations and corresponding energy laws are given. The time semi-discrete scheme is presented in Section 3, and mass conservation, unconditionally unique solvability, unconditionally energy stability and error estimate are proved rigorously. In Section 4, the mixed finite element fully discrete scheme is established. Some numerical experiments are presented to check the theoretical analysis and demonstrate the effectiveness of the proposed scheme in Section 5. Section 6 gives some conclusions.

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